

Rayleigh–Ritz variation method and connected–moments polynomial approach

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Abstract

We show that the connected–moments polynomial approach proposed recently is equivalent to the well known Rayleigh–Ritz variation method in the Krylov space. We compare the latter with one of the original connected–moments methods by means of a numerical test on an anharmonic oscillator.

1 Introduction

The t –expansion [1] has motivated a great interest in the application of the connected–moments expansion (CMX) [2] and its variants [3–5] to quantum–mechanical models. In spite of its limitations [3–8] the CMX has proved useful for the study of many physical problems [2, 3, 6, 7, 9–12].

Recently, Bartashevich [13] proposed the connected–moments polynomial approach (CMPA) that yields approximate eigenvalues to all states as roots of a simple polynomial function of the energy with coefficients that depend on the moments of the Hamiltonian operator.

The purpose of this paper is to show that the CMPA is simply the Rayleigh–Ritz variation method (RRVM) [14] in a Krylov subspace.

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2 Rayleigh–Ritz variation method and connected–moments polynomial approach

It is our purpose to solve the eigenvalue equation

$$\hat{H} |\psi_j\rangle = E_j |\psi_j\rangle, \quad j = 0, 1, \dots \quad (1)$$

by means of the RRVM [14] in the Krylov space spanned by $\{|\phi_j\rangle = \hat{H}^j |\phi\rangle\}_{j=0}^{\infty}$, where $|\phi\rangle$ is a properly chosen vector of the state space. The RRVM makes the trial function

$$|\varphi\rangle = \sum_{j=0}^{N-1} c_j |\phi_j\rangle \quad (2)$$

orthogonal to the subspace spanned by $\{|\phi_j\rangle = \hat{H}^j |\phi\rangle\}_{j=0}^{N-1}$; that is to say:

$$\langle\phi_j| (\hat{H} - W) |\varphi\rangle = 0, \quad j = 0, 1, \dots, N-1 \quad (3)$$

where W is one of the RRVM roots and an approximation to the corresponding eigenvalue. The coefficients c_j are solutions to the secular equations

$$\sum_{i=0}^{N-1} (H_{ji} - W S_{ji}) c_i = 0, \quad j = 0, 1, \dots, N-1 \quad (4)$$

where the matrix elements $H_{ji} = \langle\phi_j| \hat{H} |\phi_i\rangle = \mu_{i+j+1}$ and $S_{ji} = \langle\phi_j| \phi_i\rangle = \mu_{i+j}$ are given in terms of the moments $\mu_j = \langle\phi| \hat{H}^j |\phi\rangle$. There are nontrivial solutions to the homogeneous system of linear equations (4) only for the N values of $W = W_0, W_1, \dots, W_{N-1}$ that are roots of the secular determinant

$$|\mu_{i+j+1} - W \mu_{i+j}|_{i,j=0}^{N-1} = 0. \quad (5)$$

It is well known that the RRVM approximate eigenvalues approach the exact ones from above: $W_n^{[N]} > W_n^{[N+1]} > E_n$, $n = 0, 1, \dots, N-1$ [14]. This statement is not valid if by chance $\langle\phi| \psi_i\rangle = 0$ because $\langle\phi_j| \psi_i\rangle = 0$, $j = 0, 1, \dots$, and the eigenvector $|\psi_i\rangle$ is bypassed by the method because it is orthogonal to the Krylov space. Here we assume that the RRVM converges, criteria for the convergence of the approach have been discussed elsewhere [15].

It follows from (3) that $\langle \phi_j | \varphi \rangle = W^j \langle \phi | \varphi \rangle$, which, by virtue of (2), enables us to write

$$\langle \phi | \varphi \rangle \sum_{j=0}^N p_j W^j = \sum_{i=0}^{N-1} c_i \left(\sum_{j=0}^N p_j \mu_{i+j} \right) \quad (6)$$

and we conclude that if the coefficients p_j satisfy

$$\sum_{j=0}^N p_j \mu_{i+j} = 0, \quad i = 0, 1, \dots, N-1 \quad (7)$$

then

$$\sum_{j=0}^N p_j W^j = 0. \quad (8)$$

It is clear that we can arbitrarily choose $p_0 = 1$ and that the remaining coefficients p_j , $j = 1, 2, \dots, N$ are identical to the x_{N-j+1} of Bartashevich [13].

Since equation (8) is satisfied by all the RRVM roots, we conclude that it is exactly the characteristic polynomial that results from the secular determinant (5). In other words, the CMPA is equivalent to the RRVM which explains why the CMPA sequences converge from above [13].

In our opinion, solving the well known determinantal equation (5) is probably easier than solving equations (7) and (8) of Bartashevich's CMPA.

If we consider the N equations (7) plus (8) as a whole system of $N+1$ equations with $N+1$ unknowns p_0, p_1, \dots, p_N , then we conclude that there will be nontrivial solutions provided that

$$\begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_N \\ \mu_1 & \mu_2 & \cdots & \mu_{N+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{N-1} & \mu_N & \cdots & \mu_{2N-1} \\ 1 & W & \cdots & W^N \end{vmatrix} = 0 \quad (9)$$

which is exactly the determinantal equation derived earlier by Bishop et al [16].

It is interesting to compare the original CMX approaches with the Rayleigh-Ritz variation method in the Krylov space discussed above. For concreteness, we arbitrarily choose the so-called CMX-LT [3]. Fig 1 shows $\log |E_{approx} - E_{exact}|$

for the ground state of the dimensionless strongly-anharmonic oscillator $\hat{H} = -d^2/dx^2 + x^8$. In both cases we chose the trial function $\langle x | \phi \rangle = e^{-ax^2}$, where $a = 8$, and calculated the “exact” eigenvalue $E_0 = 1.225820113800492191$ by means of the Riccati–Padé method that exhibits remarkable rate of convergence for this kind of models [17]. We appreciate that the RRVM converges smoothly from above while the CMX–LT exhibits great oscillation. The same situation takes places for other values of a .

3 Conclusions

We have shown that the CMPA is equivalent to the RRVM. Consequently it applies to all the states and produces sequences of roots that converge from above. Numerical difficulties in applications of the CMX have been attributed to singularities in the Hankel matrix of connected moments which may not be invertible [4]. On the other hand, the Hankel matrix of moments that appear in the calculation of the coefficients x_j [13] (or present p_j ’s given by (7)) is always invertible. This is not surprising because one does not expect the RRVM to exhibit such kind of singularities. A numerical test on a simple anharmonic oscillator suggests that the RRVM may be more reliable than the CMX approaches.

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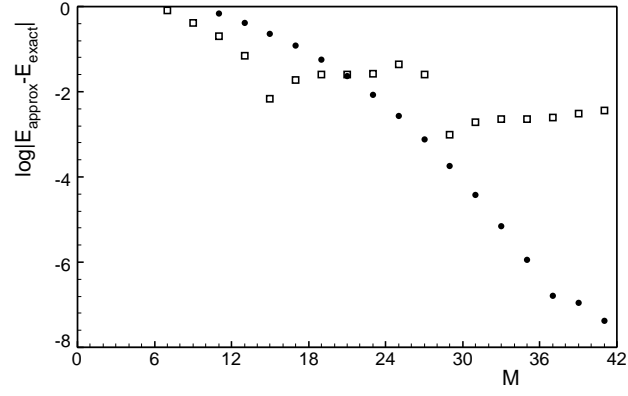


Figure 1: Rate of convergence measured as $\log|E_{approx} - E_{exact}|$ for the CMX-LT (squares) and RRVM (filled circles) in terms of the required number of moments M